Solve-o-Matic Top-Level Use Case

Version: 0.1 18/SEP/09

Introduction

The aim of this document is to provide the top-level use cases for Solve-o-Matic, with the aim of putting the derived specifications in context.

Actors

- User: the user who will most likely be either at the beamline or operating the beamline remotely. In the first instance this will be targetted at the needs of high-throughput users, namely industrial users and those from large, well organised academic labs.
- ISPyB: the beamline information management system, which holds the sample information and should ideally be populated prior to the experiment with the sample metadata (projects, sequences, models, protein names and so on) and experimental metadata during the experiment.
- GDA: the generic data acquisition system, which is used to perform the experiment, controls the experimental hardware and interacts with ISPyB.
- Cluster: this is the Sun Grid Engine managed compute cluster where the necessary computation can be performed.

Before the Experiment / Visit

The user should populate ISPyB with the sample metadata for those samples which will be analysed during the experiment. This may include the sample positions in the pucks if they are pre-mounted, and should include a protein name, which will be used to associate the sample with the expected content, either in the form of a protein sequence or model. For cases where the sample has been modified to allow experimental phasing, the modifications should also be stored.

If the putative spacegroup and cell constants are known before the experiment it may be beneficial to assign them at this stage, as this information may be used to inform decisions about the data reduction and phasing.

During the Experiment

During the experiment the sample information may be obtained to inform the correct procedures which should be performed at the end of each data collection run. At the moment we have the cabability to launch a data reduction run after each data collection: by interrogating ISPyB this could determine the best route to take for postprocessing the measurements. The links to ISPyB will also be used to record the results of the data processing and downstream structure solution.

In addition to the automated-but-simple processing it may be desirable to have the user specify data reduction and structure solution tasks from the history tab in GDA: this will need to be specified externally.

The aim is that users may be able to obtain the results of the experiment in the form of an electron density map rather than diffraction images or reduced data within a few minutes of the experiment.

For remote users there is a secondary benefit: they may be able to take the reduced data or maps and perform analysis at home, without having to ship the raw data.

After the Experiment

Once the experiment is complete the results of all of the data collection, data reduction and structure solution should be available through ISPyB. This will allow the users to have a permanent record of all of the results of the visit, which may inform the choices made during subsequent visits.